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On joint application of atomic force microscopy and light scattering data for determination of growth rate for fractal solid state surface height

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Determination of parameters for kinetic equations is one of the main problems of modern nanoengineering [1]. This report deals with estimation for the rate v of epitaxial growth of solid state surface in the framework of the simplified Kardar-Parisi-Zhang model:

$$\frac{\partial H}{\partial t} = v + \frac{v}{2} \cdot (\nabla H)^2, \tag{1}$$

where $H(\vec{x},t)$ is the height of solid state surface, $\vec{x} = (x_1, x_2)$ is two-dimensional vector of transversal coordinates and ∇ is two-dimensional gradient.

This model differs sharply from the primordial Kardar-Parisi-Zhang model suggested in article [2] because of in equation (1) there are no terms describing the surface diffusion of sputtering substance and the external source of sputtering particles. On the other hand absence of these terms gives one a possibility to solve the following problem namely let initial condition for equation (1) possesses by the next form:

$$H_0(\vec{x}) = h_0(\vec{x}) + \mu \cdot u_0(\vec{x}), \tag{2}$$

where μ is small parameter: $0 < \mu << 1$ and $u_0(\vec{x})$ is stationary stochastic two-dimensional field with zero average: $< u_0(\vec{x}) >= 0$, generally speaking $u_0(\vec{x})$ being fractal function.

Representation (2) for initial condition means that in order to construct solution of equation (1) one ought to use perturbation theory:

$$H(\vec{x},t) = h(\vec{x},t) + \mu \cdot u(\vec{x},t) + \ldots. \tag{3}$$

Further if one chooses regular shape $h_0(\vec{x})$ in initial condition (2) as follows:

$$h_0(\vec{x}) = h_* - \frac{\vec{x}^2}{2 \cdot L_*}, \tag{4}$$

(h_* and L_* are constant positive values), then zero order approximation in asymptotic series (3) is equal to:

$$h(\vec{x},t) = h_* + v \cdot t - \frac{\vec{x}^2}{2 \cdot (L_* + v \cdot t)} \tag{5}$$

(it is easy to check that function $h(\vec{x},t)$ is exact solution of equation (1)).

Thus the first order approximation in asymptotic series (3) in accordance with formula (5) ought to obey to the next linear partial differential equation with variable coefficients:

$$\frac{\partial u}{\partial t} + \frac{v \cdot \vec{x}}{L_* + v \cdot t} \cdot \nabla u = 0. \tag{6}$$

One can derive exact solution of the Cauchy problem for equation (6) with initial condition $u_0(\vec{x})$ by the well-known method of characteristics:

$$u(\vec{x},t) = u_0\left(\frac{L_* \cdot \vec{x}}{L_* + v \cdot t} \right). \tag{7}$$

It is obvious that $< u(\vec{x},t) >= 0$ therefore $< H(\vec{x},t) >= h(\vec{x},t)$. It means that one can directly calculate covariance function of total height $H(\vec{x},t)$ of solid state surface:

$$B(\vec{\xi},t) = < (H(\vec{x},t) - < H(\vec{x},t) >) \cdot (H(\vec{x}+\vec{\xi},t) - < H(\vec{x}+\vec{\xi},t) >) >, \quad (8)$$

namely if process of epitaxy lasts from $t = 0$ to $t = t_*$ then it is necessary to measure shapes $H_0(\vec{x})$ and $H(\vec{x},t_*)$ by means of atomic force microscopy before the beginning and after the end of technological process. Further one should estimate $< H_0(\vec{x}) >$ and $< H(\vec{x},t_*) >$ with help of tresholding. Tresholding is known to be a kind of denoising procedure in the framework of wavelet analysis [3].

At last one ought to derive the two-dimensional Fourier-transform from function (8):

$$S(\vec{q},t) = \int B(\vec{\xi},t) \cdot \exp(-i \cdot \vec{q} \cdot \vec{\xi}) \cdot d^2\xi \quad . \quad (9)$$

On the other hand one can measure at $t = t_*$ bistatic cross-section σ of monochromatic visible light with fixed polarization on this surface and extract from this value spectral density (9) because of the so-called small-scales approximation in this situation is valid [4].

If these functions are close in some norm then conjecture about validity of equation (1) is true hence in this case using formulae (3) and (7) it is easy to find that

$$B(\vec{\xi},t) = \mu^2 \cdot K_0\left(\frac{L_* \cdot \vec{\xi}}{L_* + v \cdot t}\right) + o(\mu^2) \quad , \quad (10)$$

$$K_0(\vec{\xi}) = < u_0(\vec{x}) \cdot u_0(\vec{x}+\vec{\xi}) > \quad (11)$$

being autocorrelated function of stochastic field $u_0(\vec{x})$.

Thus spectral density for covariance function (10) is equal to:

$$S(\vec{q},t) = \mu^2 \cdot \left(\frac{L_* + v \cdot t}{L_*}\right)^2 \cdot S_0\left(\frac{L_* + v \cdot t}{L_*} \cdot \vec{q}\right) + o(\mu^2) \quad , \quad (12)$$

where $S_0(\vec{q})$ is spectral density corresponding to autocorrelated function (11) therefore in accordance with small-scales theory [4]:

$$\frac{\sigma_{\vec{q}=0,t=t_*}}{\sigma_{\vec{q}=0,t=0}} = \left(1 + \frac{v \cdot t_*}{L_*}\right)^2 + O(\mu) \quad . \quad (13)$$

Formula (13) means that if one can measure bistatic cross-section on this surface before the start of technological process too and determine parameter L_* from expression (4) by fitting of data of atomic force microscopy after thresholding then one can estimate the rate v of epitaxial growth of solid state surface.

Quantum mechanical mechanisms of arising of two-dimensional Weierstrass-like shapes $u_0(\vec{x})$ are also considered according to approaches of article [5].

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